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# Quantization of the Aharonov-Bohm Flux threading through a Charge Density Wave Loop

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## Abstract

At low temperatures, quasi-one-dimensional conductors exhibit the charge density wave (CDW). In this paper, it is found that the CDW in the one-dimensional loop, which is the commensurate CDW, yields a quantization of the Aharonov-Bohm magnetic flux threading through the loop.

## Text

The quasi-one-dimensional conductor exhibits, at the critical temperature  $T_c(>0)$ , the charge density wave (CDW) transition [1][2][3]. Below  $T_c$ , the conductor is in the superconducting phase resulting from the CDW electronic state [4]. The CDW transition is accompanied with the Peierls structural transition, a lattice distortion with a period equal to  $\pi/k_F$  [5]. As is well-known, the interaction between electrons and phonons is responsible for this transition. In this paper, we propose the quantization of the Aharonov-Bohm magnetic flux (A-B flux) threading through a quasi-one-dimensional loop where the conduction electrons (and lattice ions) are in the CDW state.

Let us consider a one-dimensional loop which winds round an infinitely long, closely wound solenoid. The magnetic field developed by an external current source is  $\mathbf{B} = B\mathbf{e}_z$  in the solenoid, running along the polar axis. If the winding of the solenoid can be viewed as a current sheet, the magnetic field vanishes on the outside. Thus we have an A-B vector potential

$$\mathbf{A}(r, \theta) = \left(0, \frac{\Phi}{2\pi r} \mathbf{e}_\theta\right) \quad (1)$$

in  $r \geq a$  where  $a$  is a radius of the solenoid. The magnetic flux  $\Phi$  given in (1) is  $\Phi = \int_S \mathbf{B} \cdot d\mathbf{s} = \oint \mathbf{A} \cdot d\mathbf{l}$  where  $\int_S \cdots d\mathbf{s}$  and  $\oint \cdots d\mathbf{l}$  are respectively the surface and the line integrals bounded by the loop considered, and  $\mathbf{e}_\theta$  is a unit vector in the direction of the azimuthal angle  $\theta$ . We notice that our vector potential yields  $\mathbf{B} = \nabla \times \mathbf{A} = 0$  in  $r \geq a$ . The Hamiltonian of a free electron orbiting around the A-B flux is

$$H_{f,e} = \frac{1}{2m} [-i\hbar \nabla - e\mathbf{A}]^2. \quad (2)$$

The wave function  $\Psi(\mathbf{r}, t)$  satisfying the Schrodinger equation  $i\hbar\partial\Psi/\partial t = H_{f,e}\Psi$  is factorized as (here the time-dynamical vector potential is adopted for convenience)

$$\Psi(\mathbf{r}, t) = \exp[ie \int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{A}(\mathbf{r}', t) d\mathbf{r}'/\hbar] \psi(\mathbf{r}, t). \quad (3)$$

The factorized phase factor is called the Dirac phase, and the pseudo-wave function  $\psi(\mathbf{r}, t)$  satisfies the pseudo-Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = [-\frac{\hbar^2}{2m} \nabla^2 - e \int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{E}(\mathbf{r}', t) d\mathbf{r}'] \psi(\mathbf{r}, t), \quad (4)$$

where  $\mathbf{E}$  is the electric field,  $\mathbf{E} = -\partial\mathbf{A}/\partial t$ . On combining (4) with Faraday's law  $\oint \mathbf{E} d\mathbf{r} = -\partial\Phi(t)/\partial t$ , we find the multi-valued circular condition [6]:

$$\psi(r, \theta + 2\pi, t) = \exp[-2\pi i \alpha(t)] \psi(r, \theta, t), \quad (5)$$

where  $\alpha(t)$  is a scaled magnetic flux,  $\alpha(t) = e\Phi(t)/h$ .<sup>1</sup> As seen from (5),  $\alpha(t)$  can be restricted to  $-1/2 \leq \alpha(t) \leq 1/2$  without losing generality. Furthermore  $\alpha(t) > 0$  can be imposed on  $\alpha(t)$ , because the sign of  $\alpha(t)$  simply reflects the direction of the magnetic flux  $\Phi$  running along  $z$ -axis. Thus  $0 \leq \alpha(t) \leq 1/2$  will be assumed in the following. For the time-static  $\alpha$ ,  $\psi(\mathbf{r}, t)$  and the energy spectrum of the free electron confined in a loop of a radius  $r$  are respectively given from (4) and (5) as

$$\psi(\theta, t) = \frac{1}{\sqrt{2\pi r}} \exp\left[\frac{-i\epsilon_{n,\alpha}t}{\hbar}\right] \exp[i(n - \alpha)\theta] \quad (6)$$

and

$$\epsilon_{n,\alpha} = \frac{\hbar^2}{2m} k_{n,\alpha}^2 \quad (7)$$

with

$$k_{n,\alpha} = \frac{n - \alpha}{r}. \quad (8)$$

Here  $n$  is an integer,  $n = 0, \pm 1, \pm 2, \pm 3, \dots$ . Let us note that  $\psi(\theta, t)$  given in (6) satisfies the circular condition (5).

The Peierls structural transition in a quasi-one-dimensional conductor [5] is linked to the singular behavior in the time-static 1-D susceptibility [7][8]

$$\chi_1^0(q) = \sum_k \frac{f(E_k) - f(E_{k+q})}{E_{k+q} - E_k}, \quad (9)$$

where  $f(E_k)$  is the Fermi distribution function,  $f(E) = [\exp \beta(E - \mu) + 1]^{-1}$ . To calculate  $\chi_1^0(q)$ , we will neglect, for the sake of simplicity, the effects of the time-static lattice potential, and so employ the energy spectrum (7) as  $E_k$ . On replacing the summation  $\sum_k$  by an integral  $(L/2\pi) \int_{-k_F}^{k_F} dk$  ( $k \equiv n/r$ ), we have, at  $T = 0$ ,

$$\chi_1^0(q) = \frac{Lm}{2\pi\hbar^2} \frac{1}{q} \left[ \ln \left| \frac{2(k_F - \frac{\alpha}{r}) + q}{2(k_F - \frac{\alpha}{r}) - q} \right| + \ln \left| \frac{2(k_F + \frac{\alpha}{r}) + q}{2(k_F + \frac{\alpha}{r}) - q} \right| \right]. \quad (10)$$

<sup>1</sup>An extra phase  $-2\pi\alpha(t)$  of  $\psi(r, \theta + 2\pi, t)$  is cancelled out by another acquired phase  $+2\pi\alpha(t)$  which arises from the Dirac phase. Hence the wave function  $\Psi(\mathbf{r}, t)$  is single-valued for an arbitrary value of  $\alpha(t)$  [5].

In the above expression,  $k_F = n_F/r$  is the Fermi wave vector ( $n_F$  is an integer) defined by the Fermi energy  $\epsilon_F = \hbar^2 k_F^2 / 2m$  and  $L$  is the circumference of the loop,  $L = 2\pi r$ . We notice that the expression (10) is, as expected, symmetric with respect to a reflection  $\alpha \leftrightarrow -\alpha$ . At  $q = Q_\alpha = 2(n_F + \alpha)/r$  or  $q = Q_{-\alpha} = 2(n_F - \alpha)/r$ , our  $\chi_1^0(q)$  becomes singular. This implies that the system undergoes the CDW transition if the electron-phonon interactions are switched on and the temperature is lowered. The spatial wave length of the CDW is  $\lambda_\alpha = 2\pi/Q_\alpha$  or  $\lambda_{-\alpha} = 2\pi/Q_{-\alpha}$ . The wave length  $\lambda_\alpha$  ( $\lambda_{-\alpha}$ ) must satisfy the condition that the ratio  $L/\lambda_\alpha = rQ_\alpha$  ( $L/\lambda_{-\alpha} = rQ_{-\alpha}$ ) is an integer. This is expected from the common assumption that the entire wave functions composed of many conduction electrons are single-valued.<sup>2</sup> It is readily seen from the single-valuedness assumed here that the permitted values of  $\alpha$  are the quantized ones, that is,  $\alpha = 0$  and  $\alpha = 1/2$ . The state with  $Q_0$  ( $\alpha = 0$ ) is, as shown below with use of the mean-field theory, more favorable energetically than the state with  $Q_{+1/2}$  and the state with  $Q_{-1/2}$  ( $\alpha = 1/2$ ). Therefore the state with  $\alpha = 0$  is expected to be the ground state, and other two states with  $\alpha = 1/2$  are classified into the excited states.

The much simplified theory for the CDW is the mean-field treatment described by the Hamiltonian [3][4]

$$\begin{aligned}
 H_{CDW}^{\pm\alpha} = & \sum_{|n| \leq rQ_{\pm\alpha}} \epsilon_{k'} a_{k'}^\dagger a_{k'} + \sum_{0 \leq n \leq rQ_{\pm\alpha}} \Delta_{\pm\alpha}^* a_{k'-Q_{\pm\alpha}}^\dagger a_{k'} \\
 & + \sum_{-rQ_{\pm\alpha} \leq n \leq 0} \Delta_{\pm\alpha} a_{k'+Q_{\pm\alpha}}^\dagger a_{k'}, \quad (\alpha = 0, \frac{1}{2})
 \end{aligned} \quad (11)$$

where  $a_{k'}^\dagger$  and  $a_{k'}$  are respectively creation and annihilation operators of electrons, and  $k_{n,\alpha}$  given by (8) are abbreviated by  $k'$ . The pairing energy  $\Delta_{\pm\alpha}$  will be determined by the so-called gap equation (see (18)). The sum on integers  $n$  is not over the Brillouin zone  $|n| \leq n_G$  but over  $|n| \leq rQ_{\pm\alpha} \simeq 2n_F$  because the electrons with momenta  $k \simeq k_F$  are concerned with the transition. Here it should be kept in mind that the numbers of the occupied states,  $rQ_{\pm\alpha} + 1 = 2n_F \pm 2\alpha + 1$  ( $\alpha = 1/2$ ), considered in (11) differ from the actual number of the occupied states  $2n_F + 1$  given from  $|n| \leq n_F$ . That is to say, the empty state  $n = -(n_F + \alpha)$  is superfluously occupied by two extra electrons in the case of  $H_{CDW}^{+\alpha}$ , while the two electrons at  $n = n_F + \alpha$  have been illegally excluded from  $H_{CDW}^{-\alpha}$  ('two electrons' is due to the two spin states at a given  $n$ ). Therefore the special notice will be taken when the energy for  $H_{CDW}^{+\alpha}$  or  $H_{CDW}^{-\alpha}$  is calculated (see (15) and (17)).

With the aids of  $\tilde{k} \equiv k' - Q_{\pm\alpha}/2$  and  $\tilde{k} \equiv k' + Q_{\pm\alpha}/2$  respectively introduced for  $0 \leq n \leq rQ_{\pm\alpha}$  and for  $-rQ_{\pm\alpha} \leq n \leq 0$ ,  $H_{CDW}^{\pm\alpha}$  can be converted into

$$\begin{aligned}
 H_{CDW}^{\pm\alpha} = & \sum_{|\tilde{n}| \leq rQ_{\pm\alpha}/2} (a_{\tilde{k}+Q_{\pm\alpha}/2}^\dagger, a_{\tilde{k}-Q_{\pm\alpha}/2}^\dagger) \\
 & \times \begin{pmatrix} \epsilon_{\tilde{k}+Q_{\pm\alpha}/2} & \Delta_{\pm\alpha} \\ \Delta_{\pm\alpha}^* & \epsilon_{\tilde{k}-Q_{\pm\alpha}/2} \end{pmatrix} \begin{pmatrix} a_{\tilde{k}+Q_{\pm\alpha}/2} \\ a_{\tilde{k}-Q_{\pm\alpha}/2} \end{pmatrix},
 \end{aligned} \quad (12)$$

<sup>2</sup>For a free particle moving in the A-B potential the wave function, as given in the former footnote, is *proved* to be single-valued. Contrary to this, the single-valuedness of the wave functions for many-body systems has not been proved as yet, so that it is regarded as an assumption.

where the integers  $\tilde{n}$  are defined by

$$\tilde{k} \equiv \frac{\tilde{n} - \alpha}{r} \quad (13)$$

for both  $Q_{\pm\alpha}$ . The integers  $\tilde{n}$  are in accordance with the integers  $n$  in (8). Diagonalizing the above  $2 \times 2$  matrix, we have the eigenvalues

$$E_{\pm}^{\pm\alpha}(\tilde{k}) = \frac{\hbar^2}{2m} \left\{ \tilde{k}^2 + \left( \frac{Q_{\pm\alpha}}{2} \right)^2 \right\} \pm \left\{ \left( \frac{\hbar^2}{2m} \tilde{k} Q_{\pm\alpha} \right)^2 + |\Delta_{\pm\alpha}|^2 \right\}^{\frac{1}{2}}. \quad (14)$$

The energy for  $Q_{+\alpha}$  ( $\alpha = 0, 1/2$ ) is, at  $T = 0$ , given by

$$E_{CDW}^{+\alpha} = 2 \sum_{|\tilde{n}| \leq n_F + \alpha} E_{-}^{+\alpha}(\tilde{k}) - 4\alpha E_{-}^{+\alpha}(-\frac{\alpha}{r}). \quad (15)$$

The summation spans over the whole states  $|n| \leq n_F + \alpha$ , because after the transition all electrons considered in (11) condense in the states lying under the opened gap  $2|\Delta_{+\alpha}|$ . The energy  $E_{-}^{+\alpha}(-\alpha/r)$  is the one of the quasi-particle at  $\tilde{n} = 0$  or equivalently at  $n = -(n_F + \alpha)$ . The reason why this term is subtracted is, as was mentioned below (11), that the empty state  $n = -(n_F + \alpha)$  is superfluously counted as the occupied state in the Hamiltonian  $H_{CDW}^{+\alpha}$ . A coefficient  $4\alpha$  in front of  $E_{-}^{+\alpha}(-\alpha/r)$  implies that this term should disappear in the case of  $\alpha = 0$ . Replacing  $\sum_{|\tilde{n}| \leq n_F + \alpha}$  by  $(L/2\pi) \int_{-k_F - \alpha/r}^{k_F + \alpha/r} d(\tilde{n}/r) = (L/2\pi) \int_{-k_F - 2\alpha/r}^{k_F} d\tilde{k}$ , we obtain, to lowest order in the small parameters  $|\Delta_{+\alpha}|/\epsilon_F$  and  $\alpha/n_F$  ( $rk_F = n_F$ ),

$$\begin{aligned} E_{CDW}^{+\alpha} = & 2n_F \left[ \frac{2}{3}\epsilon_F - \frac{|\Delta_{+\alpha}|^2}{4\epsilon_F} - \frac{|\Delta_{+\alpha}|^2}{2\epsilon_F} \ln\left(\frac{4\epsilon_F}{|\Delta_{+\alpha}|}\right) \right] \\ & + 4\alpha \left[ \left\{ \left( \frac{2\alpha}{n_F}\epsilon_F \right)^2 + |\Delta_{+\alpha}|^2 \right\}^{\frac{1}{2}} - \frac{2\alpha}{n_F}\epsilon_F \right]. \end{aligned} \quad (16)$$

The last term added in (16) is  $\simeq 4\alpha n_F |\Delta_{+\alpha}|^2/\epsilon_F$  for  $2\alpha/n_F \gg |\Delta_{+\alpha}|/\epsilon_F$ , and  $\simeq 4\alpha |\Delta_{+\alpha}|$  for the inverse limit  $2\alpha/n_F \ll |\Delta_{+\alpha}|/\epsilon_F$ . The energy for  $Q_{-\alpha}$  ( $\alpha = 0, 1/2$ ) is, at  $T = 0$ , given by

$$E_{CDW}^{-\alpha} = 2 \sum_{|\tilde{n}| \leq n_F - \alpha} E_{-}^{-\alpha}(\tilde{k}) + 4\alpha E_{+}^{-\alpha}(\frac{\alpha}{r}). \quad (17)$$

The result calculated is obtained in (16) with  $|\Delta_{-\alpha}|$  in place of  $|\Delta_{+\alpha}|$ .

The pairing energies  $\Delta_{\pm\alpha}$  ( $\alpha = 0, 1/2$ ) are determined by the gap equation [3][4] which is given by

$$1 = 2\lambda \frac{\epsilon_F}{N_L} \sum_{|\tilde{n}| \leq n_F \pm \alpha} \frac{1}{E_{+}^{\pm\alpha}(\tilde{k}) - E_{-}^{\pm\alpha}(\tilde{k})} \quad (18)$$

at  $T = 0$ , where  $N_L$  is a number of the lattice sites in the loop and  $\lambda$  is the non-dimensional coupling constant between electrons and phonons. If one may wish, we can derive the gap equation (18) from the Hamiltonian including the phonon term. An analogous approximated calculation leading to (16) now gives

$$|\Delta_{\pm\alpha}| = 4\epsilon_F \exp\left[-\frac{1}{\lambda\nu} \left(1 \pm \frac{\alpha}{n_F}\right)\right], \quad (\alpha = 0, \frac{1}{2}) \quad (19)$$

where  $\nu \equiv 4n_F/N_L$ , and  $\alpha/n_F \ll \lambda (\ll 1)$  has been used. From the above formulas, it follows that the corrections for the pairing energies due to  $\alpha$ , namely  $\simeq \pm \alpha \Delta_0 / (n_F \lambda \nu)$ , make negligibly small contributions to the respective energies  $E_{CDW}^{\pm\alpha}$ . Thus we can replace  $\Delta_{\pm\alpha}$  by  $\Delta_0$  when the energies (15) and (17) are considered. Finally, we are led to the conclusion

$$E_{CDW}^0 < E_{CDW}^{+\frac{1}{2}} = E_{CDW}^{-\frac{1}{2}} \quad (20)$$

under the approximated calculations.

We turn now to a description of the electromagnetic response of the system. The flux  $\Phi$ , which has been shown to be quantized, is produced by an external current source of the solenoid *and* by an induced current on the loop. That is to say, an induced vector potential  $\mathbf{A}_{ind}(\mathbf{r})$  superimposed on the externally produced vector potential  $\mathbf{A}_{ext}(\mathbf{r}) = \Phi_{ext} / 2\pi r \cdot \mathbf{e}_\theta$ , leads to  $\Phi$ -quantization. The induced vector potential is determined by Maxwell's equation

$$\nabla^2 \mathbf{A}_{ind}(\mathbf{r}) = -\mu_0 \mathbf{j}_{ind}(\mathbf{r}) \quad (21)$$

where  $\mathbf{j}_{ind}(\mathbf{r})$  is a induced current density on the loop. As is discussed above, our vector potential  $\mathbf{A}$  appearing in the Hamiltonian (2) is the total vector potential  $\mathbf{A}_{tot}(\mathbf{r}) = \mathbf{A}_{ext}(\mathbf{r}) + \mathbf{A}_{ind}(\mathbf{r})$ . As to  $\mathbf{A}_{tot}(\mathbf{r})$ , it was assumed for convenience' sake that  $\mathbf{A}_{tot}(\mathbf{r})$  as well as  $\mathbf{A}_{ext}(\mathbf{r})$  is idealized into the form (1). Let us note now that the single-valuedness of the electron-ion wave function only permits the *commensurate* CDW [9] in the loop. Therefore there is a potential barrier of the commensurate pinning force [10]. If this force is substantial, it would prevent the CDW from sliding classically [11]. Here one may ask why  $\mathbf{j}_{ind}(\mathbf{r})$  is possible? The present author thinks that our  $\mathbf{j}_{ind}(\mathbf{r})$  is due to the *quantum tunneling* [12] through the potential barrier. To begin with, the one-dimensional loop considered is the mesoscopic one where the phase coherence of the wave function is expected to go round the loop. Without such a phase coherence, the Aharonov-Bohm flux can be entirely eliminated by the gauge transformation, and so the problem studied in this paper fails to materialize. In this sense, the problem is fundamentally quantum mechanical.

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